IMPRS on Multiscale Biosystems

Project title: MD simulations and multiscale modeling of specific membrane adhesion
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Project description: Biological processes involve the specific binding of molecules. These molecules are either *soluble*, i.e. free to diffuse throughout intracellular compartments or extracellular spaces, or are *anchored* to the membranes of cells or organelles. Key biological processes that are mediated by the binding of membrane-anchored molecules are the adhesion of cells or organelles in immune responses, tissue formation, and cell signaling. In contrast to soluble molecules, the binding of such membrane-anchored molecules still poses fundamental problems. Central questions are how the elasticity of the membranes and the flexibility of the molecules affect the binding equilibrium and kinetics.

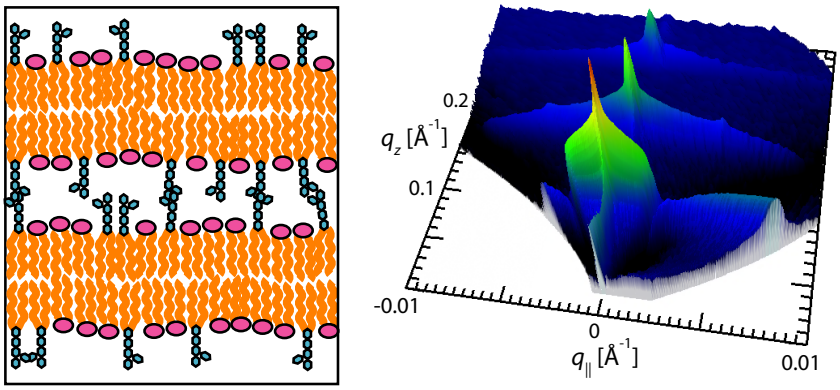

Figure: *(left) Reconstituted lipid membranes with lipid-anchored sugar molecules. - (right) Neutron scattering data from a stack of membranes interacting via lipid-anchored sugar molecules.*

In this project, we will investigate the specific binding of membrane-anchored sugar molecules with atomistic molecular dynamics (MD) simulations and statistical-physical multiscale modeling. Our central goal is the quantitative comparison to data from neutron scattering experiments that allow to measure the nanoscale separation and roughness of the apposing membranes. Besides atomistic simulations and modeling, the student working in this project will be closely involved in the analysis and interpretation of neutron scattering experiments carried out at leading international neutron sources.

Required background: M.Sc. in physical or chemical sciences, basic knowledge of statistical physics.

Papers to read before the interview: J Hu, R Lipowsky, TR Weikl. *Proc. Natl. Acad. Sci. USA* 110:15283 (2013); E Schneck, B Demé, C Gege, M Tanaka. *Biophys. J.* 100:2151 (2011).

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